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Heat and water transport in soils and across the soil-atmosphere interface – Part 1: Theory and different model concepts.

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25

26 **Abstract**

- 27 • We review theory and model concepts for evaporation from porous media.
- 28 • We discuss the underlying assumptions and simplifications of different approaches.
- 29 • Approaches differ in the description of lateral transport, transport in the air phase of the
- 30 porous medium, and coupling at the porous medium free flow interface.

31

32 **Abstract**

33 Evaporation is an important component of the soil water balance. It is comprised of water flow
34 and transport processes in a porous medium that are coupled with heat fluxes and free air flow.
35 This work provides a comprehensive review of model concepts used in different research fields to
36 describe evaporation. Concepts range from non-isothermal two-phase flow, two-component
37 transport in the porous medium that is coupled with one-phase flow, two-component transport in
38 the free air flow to isothermal liquid water flow in the porous medium with upper boundary
39 conditions defined by a potential evaporation flux when available energy and transfer to the free
40 airflow are limiting or by a critical threshold water pressure when soil water availability is limiting.
41 The latter approach corresponds with the classical Richards equation with mixed boundary
42 conditions. We compare the different approaches on a theoretical level by identifying the
43 underlying simplifications that are made for the different compartments of the system: porous
44 medium, free flow and their interface, and by discussing how processes not explicitly considered
45 are parameterized. Simplifications can be grouped into three sets depending on whether lateral
46 variations in vertical fluxes are considered, whether flow and transport in the air phase in the
47 porous medium are considered, and depending on how the interaction at the interface between the
48 free flow and the porous medium is represented. The consequences of the simplifications are
49 illustrated by numerical simulations in an accompanying paper.

50

51

52 **Introduction**

53 The primary exchanges of heat and water that motivate global and local meteorological conditions
54 occur at the Earth's surface. Many weather and climate phenomena (e.g., monsoons and droughts
55) are primarily influenced by processes associated with land-atmosphere interactions in which soil
56 moisture and its control on evapotranspiration plays an important role [*Seneviratne et al.*, 2006].
57 More than half of the Earth's surface is arid or semiarid having little to no vegetative cover [*Katata*
58 *et al.*, 2007; *Verstraete and Schwartz*, 1991; *Warren*, 1996]. In addition, over 40% of the Earth's
59 terrestrial surface is devoted to agricultural purposes, much of which, due to tillage practices, is
60 bare over a substantial period of the year. Properly describing the water cycle on the basis of heat
61 and water exchanges between the atmosphere and the soil surface is paramount to improving the
62 understanding of water balance conditions in these regions. Despite the importance of these
63 predictions, standard models vary in their ability to predict water fluxes, flow pathways and water
64 distribution. For instance, the fraction of globally averaged evaporation from the soil surface to
65 the total evapotranspiration from the land surface (i.e. including transpiration by the vegetation)
66 varies for different land surface models between 36% and 75% [*Wang and Dickinson*, 2012] with
67 a mean of 58%.

68 Understanding and controlling evaporation rates from soil is also important at much smaller scales
69 for the water management of cropped soils. For instance, in rain fed agriculture in semiarid regions,
70 where fields are cropped only once every two years and water is harvested during the non-cropped
71 year, evaporation losses during the non-cropped year determine the process or practice efficiency.
72 Evaporation may be reduced in several ways. First, by tillage, capillaries or fine pores that connect
73 the evaporating soil surface with the water stored deeper in the soil are disrupted, potentially
74 decreasing evaporation fluxes. Nevertheless, tillage may bring deeper wet soil to the soil surface
75 therefore increasing the evaporation losses. In addition, vapor diffusion may be facilitated through
76 the large interaggregate pores in tilled soils. The rougher surface of a tilled soil may also affect

77 reflectivity (albedo) and net radiation [Potter *et al.*, 1987] and the vapor transfer between the soil
78 surface and the atmosphere. Tillage-affected soil structure alter the evaporation behavior
79 depending on the weather conditions and may either lead to larger or smaller evaporation losses
80 [Moret *et al.*, 2007; Sillon *et al.*, 2003; Unger and Cassel, 1991]. Another way to reduce
81 evaporation from soil is through a drying concept known as “self-mulching”, referring to the
82 development of a dry layer within the soil, which transfers moisture only in the vapor phase [Li *et*
83 *al.*, 2016; Novak, 2010]. This naturally formed layer represents an effective way to maintain soil
84 moisture in the subsurface and it can be improved artificially by applying non-natural mulching
85 materials, such as gravel or plastic, to the soil surface in arid/semi-arid regions or in various
86 horticultural systems [Chung and Horton, 1987; Modaihsh *et al.*, 1985; Tarara and Ham, 1999;
87 Yamanaka *et al.*, 2004]. The physical mechanism is a hygroscopic equilibrium between the soil
88 vapor pressure and the atmospheric humidity, minimizing the evaporation from the mulch [Fuchs
89 and Hadas, 2011]. Several experimental studies have been conducted to investigate the effects of
90 mulch properties on soil surface evaporation processes [Diaz *et al.*, 2005; Xie *et al.*, 2006; Yuan *et*
91 *al.*, 2009]. A negative correlation between evaporation reduction ability and grain size as well as
92 a positive correlation with mulch thickness has been recognized through sensitivity analyses of
93 experimental results. Or *et al.* [2013] reviewed the physical processes that control evaporation
94 processes from porous media and focused on the role of capillary and viscous forces and of
95 diffusive transfers in the porous medium and across the interface between the porous medium and
96 the free flow. This approach allowed them to relate evaporation process to microscopic properties
97 of the porous medium. In simulation models that operate at the continuum scale, these small scale
98 processes and properties must be included in macroscopic properties and constitutive relations
99 between properties, states and fluxes.

100 Practical and theoretical limitations of modeling efforts at the continuum scale are often magnified
101 at the land-atmosphere interface, where water and energy fluxes are highly dynamic and
102 dramatically influenced by changes in temperature and moisture gradients and direction of flows

103 [Lehmann *et al.*, 2012]. The flow and transport behavior at the soil surface is affected by the
104 conditions in the atmosphere (e.g., humidity, temperature, wind velocity, solar radiation) and by
105 the soil thermal and hydraulic properties and states (e.g., thermal and hydraulic conductivity,
106 porosity, capillary pressure, temperature, vapor pressure), all of which are strongly coupled [Sakai
107 *et al.*, 2011]. For most subsurface models, the soil surface serves as the upper boundary to the
108 porous medium domain and is characterized using prescribed flux terms that serve as sources and
109 sinks. Similarly, in most atmospheric models, the vadose zone serves as a lower boundary with
110 prescribed fluxes. Such an approach is a simplification of the interaction processes at the common
111 interface of the two flow compartments. Although widely used due to its simplicity and ease of
112 use, such an approach has been shown by both atmospheric and hydrogeological scientists to
113 misrepresent flux conditions, resulting in model prediction errors [Seager *et al.*, 2007].

114 In practice, the Richards equation is the most frequently used conceptual model to describe water
115 movement within the vadose zone, and to simulate water and energy exchanges between the land
116 surface and the atmosphere at the global scale. However, it is mostly used in a form that considers
117 only isothermal liquid water flow but neglects vapor diffusion and air flow in the porous medium
118 and the effects of temperature gradients on flow and transport processes. Although the application
119 of Richards equation has been successful to describe soil water fluxes at various scales (e.g.
120 [Mortensen *et al.*, 2006; Nieber and Walter, 1981; Schoups *et al.*, 2005; Vereecken *et al.*, 1991]),
121 there may arise conditions in which the non-considered processes become relevant. The predictive
122 capacities of the Richards equation to evaluate, for instance, surface manipulations that influence
123 air flow, vapor transport and thermal regimes in the porous medium could therefore be questioned.

124 Also for global scale simulations, the consideration of additional processes such as vapor transport
125 in the soil and transport driven by thermal gradients are receiving more attention to reduce the bias
126 in bare soil evaporation predictions that are observed in these models [Tang and Riley, 2013b].

127 Most Richards equation based models assume that soil water flux is one-dimensional (i.e. water
128 flow only occurs vertically), thus neglecting any lateral variations in fluxes within the soil profiles

129 and also at the soil-atmosphere interface. Three-dimensional solutions of the Richards equation
130 have been used to investigate the effect of soil heterogeneity and hence dimensionality on flow
131 and transport processes. However, these simulation studies focused mostly on conditions when
132 flow was directed downward (infiltration). For certain problems of practical relevance, e.g.
133 evaporation from surfaces that are partially covered by mulches or row crops, a multidimensional
134 description of upward flow in the soil is used [Bristow and Horton, 1996; Horton, 1989]. The few
135 studies that also looked at heterogeneous flow and transport for upward directed flow
136 (evaporation) reported conceptual problems with the definition of the boundary conditions at the
137 soil surface [Bechtold *et al.*, 2012; Schlüter *et al.*, 2012].

138 Boundary conditions for the Richards equation are determined as a uniform flux boundary
139 condition, which is derived by solving a surface energy balance, as long as a threshold pressure
140 head is not reached. When the soil dries out and the critical pressure head is reached, the boundary
141 condition is switched to a pressure head boundary condition. First, the definition of this critical
142 pressure head is often debated. Second, for a heterogeneous soil surface in which patches of wet
143 soil alternate with dried out areas, the evaporation rate from the wet patches may increase
144 compared to the evaporation from a uniformly wet surface due to lateral exchange processes in the
145 air flow (free flow) or in the porous medium. The effect of lateral exchange processes in the free
146 flow on evaporation leads to the so-called ‘oasis effect’ and has been quantified to evaluate, for
147 instance, the effect of the size of pores [Assouline *et al.*, 2010; Shahraeeni and Or, 2012],
148 evaporation pans [Brutsaert and Yu, 1968], or ponds and lakes [Harbeck, 1962]. Lateral water and
149 heat fluxes in heterogeneous porous media may lead to a larger water loss due to evaporation from
150 a porous medium compared to the water loss from a homogeneous medium [Lehmann and Or,
151 2009; Shahraeeni and Or, 2011].

152

153 The general objective of this paper is to theoretically compare various model concepts used to
154 describe evaporation processes from soils at the continuum scale. Modeling concepts vary in

155 complexity from fully coupled free flow and porous media flow representations to reduced
156 complexity models such as those using Richards equations. First, we present the modeling
157 concepts for flow and transport in the porous medium (i.e. soil), the free flow (i.e. atmosphere),
158 and the coupling of the porous medium with the free flow (Figure 1). As different scientific
159 communities (soil physics, hydrology, atmospheric sciences and micrometeorology, and fluid
160 mechanics in porous media and in free flow) place different emphasis on the porous medium versus
161 the free flow, oftentimes the coupling is strongly simplified or overlooked. This often leads to
162 inconsistencies in the degree of detail with which processes are described in the porous medium
163 or in the free flow (e.g. 3-D flow in the porous medium coupled with a 1-D transfer resistance to
164 describe the exchange with the free flow) and misunderstandings between communities about the
165 importance of different processes. Therefore, the first objective of this work is to present a
166 comprehensive set of equations that describe all processes in both compartments (free flow and
167 porous medium) and all relevant coupling conditions. This is followed a discussion of common by
168 simplifications that lead to models of reduced complexity. Table 1, provides an overview of the
169 constitutive equations for the two compartments, their interface and potential simplifications.
170 What can be observed immediately from Table 1 is that the variables and parameters used in the
171 various approaches differ significantly.

172 The second objective is to show the similarities and differences between the different approaches
173 by deriving the variables and parameters based on a theoretical analysis of the comprehensive
174 model. Model simplifications and 'fixes' are explained in detail, thus allowing for a full
175 understanding of all approaches and for a classification of the simplifications.

176 In an accompanying paper, the consequences of these simplifications on the predictions of
177 evaporation are investigated for two sets of exemplary simulations.

178

179 **Coupled heat and water flow in porous media: overview of** 180 **concepts and simplifications at the continuum scale**

181 In this section, we introduce the model concepts used to describe heat and water fluxes in soils at
182 the continuum scale. From the general balance equations, simplified equations are derived and the
183 assumptions behind these simplifications are discussed. The employed constitutive equations are
184 presented.

185

186 **Balance equations:**

187 A full description of water and vapor transport in a porous medium requires a description of flow
188 of the two fluid phases, liquid and gas $\{l, g\}$, and of the transport of the components, water and
189 dry air $\{w, a\}$ in each of the two phases. For simplicity, we consider air as a pseudo-component
190 consisting of oxygen, nitrogen and other gases except vapor, which is regarded as separate
191 component. A mass balance for each component $\kappa \in \{w, a\}$ is given by:

$$\sum_{\alpha \in (l, g)} \phi \frac{\partial \rho_{\alpha} X_{\alpha}^{\kappa} S_{\alpha}}{\partial t} + \nabla \cdot \mathbf{F}^{\kappa} = 0 \quad [1]$$

192

193 where ϕ is the porosity, which is assumed to be constant, ρ_{α} is the mass density of phase α [kg m^{-3}], X_{α}^{κ} is the mass fraction of component κ in phase α , S_{α} is the saturation or the volume fraction
194 of the porosity occupied by phase α , \mathbf{F}^{κ} is the mass flux of component κ [$\text{kg m}^{-2} \text{s}^{-1}$]. Source and
195 sink terms (e.g. to account for liquid uptake by roots) are not included in the mass balance
196 equations but can be simply added. The component mass flux \mathbf{F}^{κ} is given by:

$$\mathbf{F}^{\kappa} = \sum_{\alpha \in (l, g)} \left(\mathbf{q}_{\alpha} \rho_{\alpha} X_{\alpha}^{\kappa} - D_{\alpha, pm}^{\kappa} \rho_{\alpha} \frac{M^{\kappa}}{\bar{M}_{\alpha}} \nabla x_{\alpha}^{\kappa} \right) \quad [2]$$

198

199 where \mathbf{q}_α [m s⁻¹] is the volume flux of phase α , $D_{\alpha,pm}^\kappa(S_\alpha)$ [m² s⁻¹] is the effective diffusion
 200 coefficient of component κ in phase α in the porous medium, x_α^κ is the molar fraction of κ in α ,
 201 M^κ is the molar mass of κ and \bar{M}_α is the mole weighted average molar mass of phase α , with $\bar{M}_\alpha =$
 202 $x_\alpha^w M^w + x_\alpha^a M^a$. The effective diffusivity is lower than the diffusivity of κ in phase α alone: D_α^κ
 203 due to the tortuosity of the diffusive pathways and the smaller cross-sectional area available for
 204 diffusion within the porous medium, which depend both on the phase saturation [Millington and
 205 Quirk, 1961]. The volume fluxes are calculated with an extended Darcy's law for multiple fluid
 206 phases:

$$\mathbf{q}_\alpha = -\frac{k_{r\alpha}(S_\alpha)}{\mu_\alpha} \mathbf{k} \cdot \nabla(p_\alpha - \rho_\alpha \mathbf{g} \mathbf{z}) \quad [3]$$

207
 208 where $k_{r\alpha}(S_\alpha)$ is the relative permeability of phase α at a saturation S_α , \mathbf{k} is the intrinsic
 209 permeability tensor [m²], μ_α [Pa s] is the dynamic viscosity of phase α , p_α [Pa] is the phase
 210 pressure, \mathbf{g} [m s⁻²] is the gravitational acceleration vector (directed downwards) and \mathbf{z} [m] is the
 211 coordinate vector (positive upward). To close the system of equations, supplementary equations
 212 need to be specified.

213 First, the capillary pressure is defined as the pressure difference between the non-wetting and
 214 wetting phase: $p_c = p_g - p_l$. According to the Young-Laplace equation capillary pressure
 215 depends on the surface tension of the gas-fluid interface, σ (N m⁻¹), and on the curvature of the
 216 gas-liquid interfaces, r (m⁻¹), which depends on the saturation degree, S_l :

$$p_c = \frac{2\sigma(T)}{r(S_l)} \quad [4]$$

217
 218 In continuum scale models, functional relations between the saturation degrees of the phases and
 219 the capillary pressure: $p_c = f(S_l)$, are used (e.g. [Brooks and Corey, 1964; van Genuchten, 1980]).
 220 Using simple pore network models, the form and parameters of relative permeability-saturation

functions were linked to the capillary pressure-saturation functions. In the Mualem van-Genuchten model, cylindrical pores are assumed. Assuming other pore geometries, e.g. triangular pores, lead to considerably higher permeabilities under dry soil conditions [Diamantopoulos and Durner, 2015; Peters and Durner, 2008; Tuller and Or, 2001]. Also, retention functions which describe the dry range of the water retention curve better than the van Genuchten function have been proposed and tested (e.g. [Lu et al., 2008]) and might be more suited to describe evaporation processes.

Second, the sum of all phase saturations and of all mass fractions equals 1.

Third, a chemical equilibrium of a component between different phases may be assumed. This sets a relation between the mole fraction of air in the liquid phase, x_l^a , and the partial air pressure p_g^a [Pa] in the gas phase using Henry's law. Furthermore, a relation between the vapor pressure and the capillary pressure is given by Kelvin's equation [Edlefsen and Anderson, 1943]:

$$p_g^w = p_{g,sat}^w \exp\left(-\frac{p_c M^w}{\rho_l R T}\right) \quad [5]$$

where $p_{g,sat}^w$ [Pa] is the temperature-dependent saturated vapor pressure, M^w is the molecular weight of water [kg mol⁻¹], R is the universal gas constant [J mol⁻¹ K⁻¹] and T [K] is the absolute temperature. The relation between the capillary pressure and the water vapor pressure only holds for dilute solutions. When the concentration of salts increases, also the osmotic soil water potential must be considered in Eq. [5] and an additional component equation for salt transport in the liquid phase and chemical equilibrium equations describing salt precipitation and dissolution must be included. We will not consider osmotic effects in the following but refer to [Nassar and Horton, 1997; 1999] who describe a model that considers coupled heat, vapor, liquid water, and solute transport. The mole fractions and partial pressures can be directly related to the mass fractions X_α^k using molar weights and the ideal gas law:

$$\rho_g X_g^w = \rho_g^w = \frac{M^w p_g^w}{RT} = \frac{M^w p_{g,sat}^w}{RT} \exp\left(-\frac{p_c M^w}{\rho_l RT}\right) \quad [6]$$

244

245 where ρ_g^w [kg m⁻³] is the mass density of the vapor. The mole fraction of vapor in the gas phase
 246 can be calculated as:

$$x_g^w = \frac{p_g^w}{p_g} \quad [7]$$

247

248 When chemical equilibrium does not hold, extra equations to describe the mass exchange of
 249 components between different phases are required [*Benet and Jouanna*, 1982; *Chammari et al.*,
 250 2008; *Nuske et al.*, 2014; *Ouedraogo et al.*, 2013; *Ruiz and Benet*, 2001; *Smits et al.*, 2011; *Trautz*
 251 *et al.*, 2015].

252 To properly approximate evaporative fluxes, it is important to account for the temperature
 253 conditions inside the porous medium. The vapor pressure and density of the air phase are two
 254 examples of temperature dependent state variables. A common assumption is that local thermal
 255 equilibrium between the gas, liquid and solid phase exists so that the temperatures in each of the
 256 three phases are equal to each other and a single energy balance equation can be used:

$$\sum_{\alpha \in \{l,g\}} \phi \frac{\partial \rho_\alpha u_\alpha S_\alpha}{\partial t} + (1 - \phi) \frac{\partial \rho_s c_s T}{\partial t} + \nabla \cdot \mathbf{F}_T = 0 \quad [8]$$

257

258 where u_α [J kg⁻¹] is the internal energy of phase α , ρ_s [kg m⁻³] is the mass density of the solid
 259 phase, c_s [J kg⁻¹ T⁻¹] is the heat capacity of the solid phase, T [K] is the absolute temperature, and
 260 \mathbf{F}_T [J m⁻² s⁻¹] is the heat flux. The internal energy is related to the enthalpy, h_α [J kg⁻¹] plus the
 261 pressure-volume work:

$$u_\alpha = h_\alpha - \frac{p_\alpha}{\rho_\alpha} \quad [9]$$

262

263 The enthalpy of the liquid phase is usually assumed to be independent of composition. The gas
 264 phase enthalpy, h_g , is calculated from the mass fractions and component enthalpies, h^k , of the dry
 265 air and water vapor components: $h_g = X_g^a h_g^a + X_g^w h_g^w$. Unlike the enthalpy of liquid water, the
 266 enthalpy of vapor also contains the latent heat of evaporation. The heat flux is described by:

$$\mathbf{F}_T = \sum_{\kappa \in \{a,w\}} \sum_{\alpha \in \{l,g\}} \left(\mathbf{q}_\alpha \rho_\alpha X_\alpha^\kappa - D_{\alpha,pm}^\kappa \rho_\alpha \frac{M^\kappa}{\bar{M}_\alpha} \nabla x_\alpha^\kappa \right) h_\alpha^\kappa - \lambda_{T,pm} \nabla T \quad [10]$$

267
 268 where $\lambda_{T,pm}$ [$\text{J m}^{-1} \text{s}^{-1} \text{K}^{-1}$] is the effective thermal conductivity under no mass flow conditions of
 269 the mixture of soil grains, liquid and gaseous phases. Mostly, relations are employed that derive
 270 $\lambda_{T,pm}$ from the volumetric liquid phase content. The parameters of these relations are a function of
 271 the texture of the porous medium, the organic matter content, and the dry bulk density [Campbell,
 272 1985; Chung and Horton, 1987; Cote and Konrad, 2005; 2009; de Vries, 1963; Lu et al., 2007;
 273 Tarnawski et al., 2000]. Under some conditions with high fluid velocities, $\lambda_{T,pm}$ is also a function
 274 of the hydromechanical dispersion and heat capacity of the flowing fluid [Campbell et al., 1994;
 275 Hopmans et al., 2002].

276 **Simplifications and fixes:**

277 In this section, we describe ways to simplify the above derived equations and include additional
 278 processes that are not considered in the constitutive equations or simplified equations (e.g.
 279 chemical and thermal non-equilibrium and turbulence induced gas phase fluxes in the porous
 280 medium).

281

282 **One component, ‘one-and-a-half’ phase equation:**

283

284 In this approach, flow of the gas phase is not simulated but diffusive transport of components in
 285 the gas phase is still considered. Processes in the gas phase are thus considered ‘half’.

286 This approach assumes that the pressure in the gas phase, p_g , is uniform and constant with time
 287 which results in the independence of the liquid phase pressure from flow in the gas phase. This
 288 assumption is justified based on the magnitude of the gas phase viscosity compared to that of the
 289 liquid phase (smaller by a factor 50). Therefore, Eq. [3] is only solved for the liquid phase and gas
 290 fluxes can be calculated directly from the change in the liquid phase saturation over time.
 291 Secondly, only the flux of the water component is considered, assuming that the water component
 292 flux is not influenced by the dry air concentrations in the two phases. For the liquid phase, this
 293 approximation hinges on the fact that the mass fraction of water in the liquid phase is close to one:
 294 $X_l^w \approx 1$. For the gas phase, the vapor pressure that is in equilibrium with the liquid phase is
 295 calculated from the capillary pressure (Eq. [5]), which depends only on the liquid phase pressure
 296 since the gas phase pressure is assumed to be constant. The vapor concentration is calculated using
 297 the ideal gas law (because $X_l^w \approx 1$) (Eq. [6]) and thus independent of the dry air concentration in
 298 the gas phase. Thirdly, it is assumed that advective fluxes of components in the gas phase can be
 299 neglected, $\mathbf{q}_g \rho_g X_g^w \approx 0$, compared with the diffusive fluxes. Finally, this approach assumes that
 300 gradients in the molar volume of the gas phase can be neglected and that the mass density of the
 301 liquid phase is constant. As a result of these assumptions, the water component flux equation (Eq.
 302 [2]) reduces to:

$$\mathbf{F}^w \approx \mathbf{q}_l \rho_l - \mathbf{D}_{g,pm}^w(S_g) \nabla \rho_g^w \quad [11]$$

303

304 The mass balance equation for water simplifies to:

$$\phi \frac{\partial \rho_g X_g^w S_g}{\partial t} + \phi \frac{\partial \rho_l S_l}{\partial t} - \nabla \cdot \left[\frac{\rho_l k_{rl}(S_l)}{\mu_l} \mathbf{k} \nabla (p_l - \rho_l \mathbf{g} \mathbf{z}) \right] - \nabla \cdot [\mathbf{D}_{g,pm}^w \nabla \rho_g^w] = 0 \quad [12]$$

305

306 This is the basic equation used by the soil physics community to describe non-isothermal liquid
 307 water flow and water vapor transport in soils. However, it is usually expressed in the following
 308 form [Milly, 1982; Saito *et al.*, 2006]:

$$\frac{\partial \theta_l}{\partial t} + \frac{\partial \theta_v}{\partial t} = \nabla \cdot \left[(\mathbf{K}_{l,\psi} + \mathbf{K}_{v,\psi}) \frac{\sigma(T)}{\sigma(T_{ref})} \nabla \psi|_{T_{ref}} + \mathbf{K}_{l,\psi} \mathbf{e}_z \right] + \nabla \cdot (\mathbf{K}_{l,T} + \mathbf{K}_{v,T}) \nabla T \quad [13]$$

309

310 where $\theta_l = \phi S_l$ is volumetric liquid water content and θ_v the water vapor content expressed in
 311 volume of liquid water ($\theta_v = \phi \rho_g^w S_g / \rho_l$), $\mathbf{K}_{l,x}$ and $\mathbf{K}_{v,x}$ are the hydraulic conductivities for liquid
 312 water flow and vapor transport, respectively, $\mathbf{K}_{x,\psi}$ [m s^{-1}] and $\mathbf{K}_{x,T}$ [$\text{m}^2 \text{K}^{-1} \text{s}^{-1}$] are the isothermal
 313 and thermal hydraulic conductivities, respectively, \mathbf{e}_z is the unit coordinate vector in the vertical
 314 direction, and $\psi|_{T_{ref}}$ (m) is the pressure head of the liquid phase at the reference temperature T_{ref} .
 315 The first term on the right hand side of Eq. [13] represents the total water flow due to pressure
 316 head gradients under isothermal conditions and due to gravity. Since the pressure head gradients
 317 are defined at a reference temperature, a standard relation between θ_l and $\psi|_{T_{ref}}$ can be used. The
 318 second term on the right hand side accounts for the total water fluxes that are generated by a
 319 thermal gradient.

320 In the following section, the relationships between the hydraulic properties \mathbf{K}_{xy} , the variables θ_l ,
 321 θ_l , $\psi|_{T_{ref}}$, and T , the fluid properties, and the effective diffusion coefficients and permeability are
 322 presented and the equality between Eqs. [12] and [13] elucidated.

323 The pressure head ψ of the water phase can be defined in terms of the capillary pressure p_c as:

$$p_c = -\psi g \rho_l \quad [14]$$

324

325 Assuming a uniform and constant gas phase pressure and liquid phase density, the water pressure
 326 gradient can be replaced by the pressure head gradient multiplied by a constant factor $g \rho_l$.
 327 Considering Eq. [4] the spatial gradient of ψ can be written as:

$$\nabla \psi(\theta_l, T) = \left. \frac{\partial \psi}{\partial \theta_l} \right|_T \nabla \theta_l + \left. \frac{\partial \psi}{\partial \sigma} \right|_{\theta_l} \frac{\partial \sigma}{\partial T} \nabla T \quad [15]$$

328 or

$$\nabla\psi(\theta_l, T) = \left. \frac{\partial\psi}{\partial\theta_l} \right|_T \nabla\theta_l + \left. \frac{\psi}{\sigma} \right|_{\theta_l} \frac{\partial\sigma}{\partial T} \nabla T \quad [16]$$

$$\nabla\psi(\theta_l, T) = \left. \frac{\partial\psi}{\partial\theta_l} \right|_T \left. \frac{\partial\theta_l}{\partial\psi} \right|_{T_{ref}} \nabla\psi|_{T_{ref}} + \left. \frac{\psi_{T_{ref}}}{\sigma(T_{ref})} \right|_{\theta_l} \frac{\partial\sigma}{\partial T} \nabla T \quad [17]$$

$$\nabla\psi(\theta_l, T) = \frac{\sigma(T)}{\sigma(T_{ref})} \nabla\psi|_{T_{ref}} + \left. \frac{\psi_{T_{ref}}}{\sigma(T_{ref})} \right|_{\theta_l} \frac{\partial\sigma}{\partial T} \nabla T \quad [18]$$

329

330 The first term of the right hand side of Eq. [16] represents the gradient in pressure head due to a
 331 gradient in the volumetric water content under isothermal conditions. Using the relationship
 332 between pressure head and volumetric water content at a reference temperature, T_{ref} , this term can
 333 be rewritten in terms of a pressure head gradient at a reference temperature (first term of Eq. [18]).
 334 The second term in Eq. [16] represents the gradient in pressure head due to a temperature gradient
 335 at a given volumetric water content θ_l . This term can also be rewritten in terms of a pressure head
 336 for a given water content θ_l at a reference temperature (Eq. [18]).

337 In a similar vein, the gradient $\nabla\rho_g^w$ can be written as:

$$\nabla\rho_g^w(\psi, T) = \left. \frac{\partial\rho_g^w}{\partial\psi} \right|_T \frac{\sigma(T)}{\sigma(T_{ref})} \nabla\psi|_{T_{ref}} + \left. \frac{\partial\rho_g^w}{\partial T} \right|_{\psi} \nabla T \quad [19]$$

338

339 Including Equations [14], [18], and [19] in Eq. [12] leads to the following equation:

$$\begin{aligned} \frac{\partial\theta_v}{\partial t} + \frac{\partial\theta_l}{\partial t} = \nabla \cdot \left[\left(\mathbf{K}_{l,\psi} + \frac{\mathbf{D}_{g,pm}^w(S_g)}{\rho_l} \frac{\partial\rho_g^w}{\partial\psi} \right) \frac{\sigma(T)}{\sigma(T_{ref})} \nabla\psi|_{T_{ref}} + \mathbf{K}_{l,\psi} \mathbf{e}_z \right] \\ + \nabla \cdot \left[\left(\mathbf{K}_{l,\psi} \frac{\psi_{T_{ref}}}{\sigma(T_{ref})} \right)_{\theta_j} \frac{\partial\sigma}{\partial T} + \frac{\mathbf{D}_{g,pm}^w(S_g)}{\rho_l} \frac{\partial\rho_g^w}{\partial T} \right] \nabla T \end{aligned} \quad [20]$$

340

341 Using the relation between the vapor density, capillary pressure and temperature (Eq. [6]) and
 342 defining the saturated vapor density $\rho_{g,sat}^w$ [kg m⁻³] and the relative humidity of the air $H_r =$
 343 $\rho_g^w / \rho_{g,sat}^w$ it follows from Eq. [20] that the conductivities in Eq. [13] are defined as:

$$K_{l,\psi} = \frac{\rho_l g k_{rl}(S_l)}{\mu_l} k \quad [21]$$

$$K_{v,\psi} = \frac{g M_w \rho_{g,sat}^w H_r}{\rho_l R T} D_{g,pm}^w(S_g) \quad [22]$$

$$K_{l,T} = K \left. \frac{\psi_{Tref}}{\sigma(T_{ref})} \right|_{\theta_l} \frac{\partial \sigma}{\partial T} \quad [23]$$

$$K_{v,T} = \frac{H_r}{\rho_l} \frac{\partial \rho_{g,sat}^w}{\partial T} D_{g,pm}^w(S_g) \quad [24]$$

344

345 Eq. [13] relies on the assumption of local thermal equilibrium. However, the temperature of the
 346 air, water and soil particles may differ due to the difference in thermal properties of these phases
 347 and rapid changes of soil surface temperatures. Therefore, it is argued that the temperature gradient
 348 in the soil air is often larger than the gradient of the mean temperature over the different phases.
 349 The effective diffusion of water vapor in soil may be larger than that of other gases since water
 350 vapor may condense and evaporate from capillary held water pockets (i.e. “liquid bridges” or
 351 “capillary islands”), thus blocking the diffusive transport of other gases [*Philip and De Vries*,
 352 1957]. These effects have been used to explain observations of enhanced vapor transport compared
 353 to Fick’s law of diffusion [*Gurr et al.*, 1952; *Rollins et al.*, 1954; *Taylor and Cavazza*, 1954]. To
 354 account for this, $K_{v,T}$ is multiplied by an enhancement factor η [*de Vries*, 1958; *Philip and De*
 355 *Vries*, 1957] described by empirical formulations (e.g. [*Campbell*, 1985; *Cass et al.*, 1984]). This
 356 approach has been widely used and accepted to calculate heat and water flow in soils (e.g. [*Hadas*,
 357 1977; *Reshetin and Orlov*, 1998; *Rose*, 1967; *Shepherd and Wiltshire*, 1995; *Sophocleous*, 1979]).
 358 However, the validity or need for vapor enhancement has been questioned [*Ho and Webb*, 1998;
 359 *Shokri et al.*, 2009; *Smits et al.*, 2013].

360 In addition to vapor enhancement, an enhancement of the liquid flow that is induced by thermal
 361 gradients has been proposed [*Noborio et al.*, 1996; *Saito et al.*, 2006]. This enhancement is
 362 attributed to the change in surface tension that results from changes in soil water composition

363 (ionic strength, concentration of organic surfactants) with temperature. Thermal enhancement is
364 accounted for by multiplying $K_{l,T}$ (Eq. [23]) by a non-dimensional empirical ‘gain factor’ ranging
365 in value from 0 to 10 [Nimmo and Miller, 1986].

366 In Eqs. [18] and [19], the gradients in the pressure head and vapor mass density were written in
367 terms of gradients in temperature and pressure head at a reference temperature assuming that the
368 change in water content with pressure head, $\frac{\partial \theta_l}{\partial \psi}$, is only a function of the surface tension, σ , and
369 temperature effects were attributed to changes in σ with temperature. But, the relationship between
370 θ_l and ψ also depends on the interaction between the solid and liquid phase (i.e. the contact angle
371 between the liquid-gas surface and the solid phase or solid phase wettability) which may also
372 change with temperature [Bachmann *et al.*, 2002]. Therefore, it is important to note that for non-
373 wettable soils temperature effects on solid-liquid phase interactions should be included in the
374 model to predict reduced evaporation from non-wettable soils or reduced water redistribution due
375 to temperature gradients in non wettable soil [Bachmann *et al.*, 2001; Davis *et al.*, 2014].

376

377 **Isothermal one component, ‘one-and-a-half’ phase equation:**

378 When water fluxes are considered over a longer period of time (i.e. multiple days), it may be
379 argued that the temporal average of the temperature gradients cancels out due to diurnal variations
380 in temperature. This also results in the temperature gradient driven fluxes canceling out [Milly,
381 1984]. Based on this assumption, the flow equation can be simplified to an isothermal equation
382 and flow due to a temperature gradient (i.e. in Eq. [13]) can be neglected so that for a 1-D flow
383 process (as routinely assumed in soils), the following equation is obtained:

384

$$\frac{\partial \theta_v}{\partial t} + \frac{\partial \theta_l}{\partial t} = \frac{\partial}{\partial z} \cdot \left[(K_{l,\psi} + K_{v,\psi}) \frac{\partial \psi}{\partial z} + K_{l,\psi} \right] \quad [25]$$

385

386 Isothermal one component one phase equation, Richards equation

387 Finally, when vapor transport is neglected, the classical Richards equation is obtained:

$$\frac{\partial \theta_l}{\partial t} = \frac{\partial}{\partial z} \cdot \left[K_{l,\psi} \frac{\partial \psi}{\partial z} + K_{l,\psi} \right] \quad [26]$$

388

389 Flow and transport processes in the atmosphere

390 In this section, the free flow balance equations are described and then possible simplifications are
391 presented and discussed.

392 Balance equations

393 In the context of evaporation processes from soils, flow conditions in the free flow are mostly
394 turbulent. Turbulent flow is usually highly irregular with chaotic fluctuations of the local velocity,
395 pressure, concentration and temperature [*Bird et al.*, 2007]. These fluctuations are caused by
396 vortices or eddies, which occur over a wide range of length scales. It is possible to simulate all of
397 these phenomena, but it requires the resolution of eddies on all scales and has therefore high
398 computational costs. To reduce these costs, turbulence can be parameterized rather than simulated
399 explicitly. The most commonly used parametrization approach is the so-called Reynolds
400 averaging. The basic assumption is that turbulent fluctuating quantities can be split in a temporal
401 average \bar{v} and a fluctuating part v' . This is called the Reynolds decomposition:

$$v_g = \bar{v}_g + v'_g, \quad p_g = \bar{p}_g + p'_g, \quad x_g^\kappa = \bar{x}_g^\kappa + x_g^{\kappa'}, \quad T = \bar{T} + T' \quad [27]$$

402 where v_g [m s⁻¹] is the gas velocity.

403 After replacing the instantaneous values in the balance equations by the sum of the average and
404 fluctuating parts, the balance equations are averaged over time. For a more detailed overview on
405 turbulence modeling and the Reynolds averaging procedure, we refer the reader to standard fluid
406 dynamic textbooks (e.g. [*Bird et al.*, 2007; *Wilcox*, 2006]). The total mass balance for the gas phase
407 is:

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot [\rho_g \overline{\mathbf{v}_g}] = 0 \quad [28]$$

408 The momentum balance is:

$$\frac{\partial(\rho_g \overline{\mathbf{v}_g})}{\partial t} + \nabla \cdot \left[\rho_g \overline{\mathbf{v}_g} \overline{\mathbf{v}_g} + \underbrace{\rho_g \mathbf{v}_g' \mathbf{v}_g'}_{\substack{\text{turbulent stress}/ \\ \text{Reynolds stress}}} + \overline{p_g} \mathbf{I} - \overline{\boldsymbol{\tau}_g} \right] - \rho_g \mathbf{g} = 0 \quad [29]$$

409 The gas phase is considered to act as a Newtonian fluid without dilatation, therefore the shear
 410 stress tensor $\boldsymbol{\tau}_g$ [kg m⁻¹ s⁻²] solely accounts for the resistance to shear deformation:

$$\boldsymbol{\tau}_g = \mu_g (\nabla \overline{\mathbf{v}_g} + \nabla \overline{\mathbf{v}_g}^T) \quad [30]$$

411 where μ_g [kg s⁻¹ m⁻¹] is the dynamic viscosity of the gas phase.

412 The component mass balance is given by:

$$\frac{\partial \rho_g \overline{X_g^\kappa}}{\partial t} + \nabla \cdot \left(\rho_g \overline{\mathbf{v}_g} \overline{X_g^\kappa} + \underbrace{\rho_g \mathbf{v}_g' X_g^{\kappa'}}_{\text{turbulent diffusion}} - D_g^\kappa \rho_g \frac{M^\kappa}{M_g} \nabla \overline{x_g^\kappa} \right) = 0 \quad [31]$$

413 and the energy balance by:

$$\begin{aligned} \frac{\partial \rho_g \overline{u_g}}{\partial t} + \nabla \cdot \left(\rho_g \overline{\mathbf{v}_g} \overline{h_g} + \underbrace{\rho_g \mathbf{v}_g' h_g'}_{\text{turbulent conduction}} - \lambda_{T,g} \nabla \overline{T} - \sum_{\kappa \in \{a,w\}} h_g^\kappa D_g^{\kappa_i} \rho_g \frac{M^\kappa}{M_g} \nabla \overline{x_g^\kappa} \right) \\ = 0 \end{aligned} \quad [32]$$

414

415 Multiplication of the turbulent fluctuations in the abovementioned balance equations (e.g. the
 416 convective portion of the momentum balance equation) leads to additional terms. Physically-
 417 speaking, these terms, although originating from the convective portion of the equation, act like
 418 additional viscous, diffusive, and conductive forces. Therefore, they are referred to as turbulent
 419 stress, turbulent diffusion, or turbulent conduction and require parameterization to properly
 420 account for the effects of turbulence. Various parameterizations of different complexity are well-
 421 established in literature. The simplest one is based on the Boussinesq assumption [Boussinesq,
 422 1872] which states that the Reynolds stress acts completely like a viscous stress so that only one
 423 unknown per balance equation remains. These unknowns are called eddy coefficients: eddy

viscosity μ_g^{turb} [kg m⁻¹ s⁻¹], eddy diffusivity D_g^{turb} [m² s⁻¹], and eddy conductivity λ_g^{turb} [W m⁻¹ K⁻¹] [Wilcox, 2006]. The most fundamental approach for calculating the eddy viscosity is based on the Prandtl mixing length:

$$-\rho_g \mathbf{v}_g' \mathbf{v}_g' = \boldsymbol{\tau}_g^{turb} = \mu_g^{turb} (\nabla \bar{\mathbf{v}}_g + \nabla \bar{\mathbf{v}}_g^T)$$

$$\mu_g^{turb} = \rho_g l_{mix}^2 \left| \frac{\partial \bar{v}_x}{\partial z} \right| \quad [33]$$

where $l_{mix} = \kappa z$ is the mixing length [m], κ is the von-Karman constant [-], z is the wall distance [m], and v_x the main velocity component [m s⁻¹]. The dynamic eddy viscosity can be converted to the kinematic eddy viscosity with:

$$\nu_g^{turb} = \frac{\mu_g^{turb}}{\rho_g} = l_{mix}^2 \left| \frac{\partial \bar{v}_x}{\partial z} \right| \quad [34]$$

In this model the kinematic eddy viscosity, ν_g^{turb} , is only a function of the flow and its turbulence, not of the fluid type itself.

In addition to the eddy viscosity, the eddy diffusivity and conductivity still need to be resolved. The most pragmatic approach is by applying the Reynolds analogy. It assumes that the same mechanisms leading to the eddy viscosity also lead to a higher mixing rate. Then the eddy diffusivity is related to the eddy viscosity by the turbulent Schmidt number:

$$D_g^{\kappa,turb} = \frac{\mu_g^{turb}}{\rho_g Sc^{turb}} \quad [35]$$

In the same way the eddy conductivity is obtained with the turbulent Prandtl number:

$$\lambda_{T,g}^{turb} = \frac{c_p \mu_g^{turb}}{Pr^{turb}} \quad [36]$$

442 The turbulent Schmidt and Prandtl numbers are often assumed to be one.

443 **Simplifications**

444 The solution of the three-dimensional balance equations in the free flow is computationally
445 demanding. To simplify the solution, it is often assumed that the mean wind speed, air temperature,
446 and relative humidity (i.e. vapor content of the air) do not change in the horizontal direction or
447 along the air stream and that their changes over time are slow. This assumption implies that the
448 momentum, vapor, and sensible heat fluxes out of the soil surface are equal to the respective fluxes
449 in the vertical direction in the air stream above the soil surface and do not change with height. This
450 generally applies for a sufficiently large upstream fetch of a homogeneous evaporating surface (no
451 lateral variations in soil water content, soil temperature, evaporation fluxes, and soil surface
452 roughness). It also implies that the vertical component of the air flow is assumed to be zero in both
453 the porous medium and the free flow, which is consistent with the one component ‘one-and-a-half’
454 phase formulation of the flow and transport process in the porous medium.

455 When the momentum transfer occurs mainly through turbulent eddies, of which the size increases
456 linearly with height, the eddy viscosity increases linearly with height so that the turbulent shear
457 stress τ_{turb} is given by:

$$\tau_{turb} = \rho_g \kappa v^* z \frac{dv_x}{dz} \quad [37]$$

458
459 where v^* [m s^{-1}] is the friction velocity and κ is the von Karman constant (≈ 0.4). It should be
460 noted that $\rho_g \kappa v^* z$ corresponds with the turbulent viscosity μ_g^{turb} in Eq. [33]. This leads to
461 logarithmic wind profiles that are generally observed in the so-called turbulent or ‘dynamic’
462 sublayer:

$$v_x(z) = \frac{v^*}{\kappa} \ln\left(\frac{z}{z_{0m}}\right) \quad [38]$$

463

where z_{0m} [m] is the momentum roughness length, which corresponds to the height above the soil surface where extrapolation of Eq. [38] predicts zero velocity. Similar logarithmic profiles are obtained for the air temperature and humidity. But, because of different interactions at the soil surface, the temperature (z_{0H}) and humidity (z_{0v}) roughness lengths differ from z_{0m} . The relationship between the different roughness lengths and characteristics of the porous medium-free flow interface are discussed in the following section.

Heat and water fluxes across the soil-atmosphere interface

The soil-atmosphere interface represents a crucial boundary between the porous medium and the free flow. In this section the coupling between transport in the atmosphere and the soil is discussed.

Coupling conditions:

The coupling of the two-phase porous-medium system with turbulent free flow involving the Reynolds-averaged Navier-Stokes equations is based on the model presented in *Mosthaf et al.* [2011] and revised in *Mosthaf et al.* [2014] and *Fetzer et al.* [2016]. It considers continuity of fluxes and a local thermodynamic equilibrium at the interface.

Mechanical equilibrium

Mechanical equilibrium is defined by the continuity of normal and tangential forces. The normal force acting on the interface from the free flow side is the sum of the inertia, pressure, and viscous forces. The normal force from the porous-medium side of the interface contains only the pressure force, since viscous forces are implicitly accounted for in Darcy's law. Hence, the mechanical equilibrium at the interface in the normal direction can be formulated as:

$$[\mathbf{n} \cdot (\{-\rho_g \mathbf{v}_g \mathbf{v}_g - \boldsymbol{\tau}_g - \boldsymbol{\tau}_g^{turb} + p_g \mathbf{I}\} \mathbf{n})]^{ff} = [p_g]^{pm} \quad [39]$$

487 The superscripts ff and pm mark the quantities at the free flow and the porous medium sides of
 488 the interface in the sequel. Eq. [39] implies that the gas phase pressure may be discontinuous across
 489 the interface due to the different model concepts (i.e. Navier-Stokes flow and Darcy flow) in the
 490 two domains. Furthermore, in addition to considering the normal forces, the free flow requires a
 491 condition for the tangential flow velocity components. When air flows over a porous surface, there
 492 is a small macroscopic slip-velocity, which therefore calls the no-slip condition into question. For
 493 that purpose, the Beavers-Joseph [Beavers and Joseph, 1967] or Beavers-Joseph-Saffman
 494 [Saffman, 1971] condition can be employed; the latter formulation neglects the comparatively
 495 small tangential velocity in the porous medium. The proportionality between the shear stresses τ
 496 and the slip velocity at the interface can be described as:

$$\left[\left(\mathbf{v}_g - \frac{\sqrt{k_i}}{\alpha_{BJ}\mu_g} (\boldsymbol{\tau}_g + \boldsymbol{\tau}_g^{turb}) \mathbf{n} \right) \cdot \mathbf{t}_i \right]^{ff} = 0, \quad i \in \{1, \dots, d-1\} \quad [40]$$

497
 498 Here, α_{BJ} is the dimensionless Beavers-Joseph coefficient, \mathbf{t}_i is a tangential vector, and $k_i = \mathbf{t}_i \cdot$
 499 $(k\mathbf{t}_i)$ a tangential component of the permeability tensor. The Beavers-Joseph condition was
 500 originally developed for flow which is mainly tangential to the porous-medium surface and for
 501 laminar single-phase flow in both the free flow and the porous medium. Its applicability for
 502 turbulent flow conditions was analyzed by Hahn *et al.* [2002] who concluded that the slip condition
 503 for laminar and turbulent flow is the same, because the flow conditions directly at the porous
 504 surface can be expected to be laminar (viscous boundary layer) and velocities to be slow.

505
 506 The influence of the Beavers-Joseph coefficient on the evaporation rate was analyzed in various
 507 studies for different flow regimes [Baber *et al.*, 2012; Fetzer *et al.*, 2016]. For flow parallel to the
 508 interface the evaporative fluxes are often dominated by diffusion through the boundary layer
 509 normal to the interface [Haghighi *et al.*, 2013], whereas the slip velocity promotes transport along
 510 the interface.

511

512 **Chemical equilibrium**

513 Ideally, chemical equilibrium should be formulated as continuity of the chemical potential. The
 514 problem is that the assumption of mechanical equilibrium, as previously discussed, leads to a jump
 515 in gas phase pressure across the interface. This jump in gas phase pressure comes along with a
 516 jump in vapor pressure across the interface and consequently a jump in chemical potential. Hence,
 517 continuity cannot be expressed in terms of chemical potentials. Instead, it is expressed in terms of
 518 the continuity of mole fractions in the gas phase.

519 The continuity of component fluxes is given by:

$$\begin{aligned} & \left[\left(\rho_g \mathbf{v}_g X_g^\kappa - (D_g + D_g^{turb}) \rho_g \frac{M^\kappa}{M_g} \nabla x_g^\kappa \right) \cdot \mathbf{n} \right]^{ff} = & [41] \\ & - \left[\left(\rho_g \mathbf{q}_g X_g^\kappa - D_{g,pm}^\kappa \rho_g \frac{M^\kappa}{M_g} \nabla x_g^\kappa + \rho_l \mathbf{q}_l X_l^\kappa - D_{l,pm}^\kappa \rho_l \frac{M^\kappa}{M_l} \nabla x_l^\kappa \right) \cdot \mathbf{n} \right]^{pm} \end{aligned}$$

520

521 The minus sign in the flux continuity accounts for the opposed directions of the normal vector of
 522 the porous medium and the free flow domain (see Figure 1). When summing up the two
 523 components, the continuity of total mass flux is given by:

$$[\rho_g \mathbf{v}_g \cdot \mathbf{n}]^{ff} = -[(\rho_g \mathbf{q}_g + \rho_l \mathbf{q}_l) \cdot \mathbf{n}]^{pm} \quad [42]$$

524

525 **Thermal equilibrium**

526 Thermal equilibrium assumes continuity of temperature at the interface. The free flow temperature
 527 is equal to the temperature of the gas phase; in contrast, the porous medium temperature is the
 528 temperature of one REV under the assumption of local thermal equilibrium.

529 The continuity of heat fluxes is given by:

$$\left[\left(\rho_g h_g \mathbf{v}_g - (\lambda_{T,g} + \lambda_{T,g}^{turb}) \nabla T - \sum_{\kappa \in \{a,w\}} h_g^\kappa (D_g^\kappa + D_g^{turb}) \rho_g \frac{M^\kappa}{\bar{M}} \nabla x_g^\kappa \right) \cdot \mathbf{n} \right]^{ff} = \quad [43]$$

$$R_n - \left[\left(\sum_{\kappa \in \{a,w\}} \sum_{\alpha \in \{l,g\}} \left(\mathbf{q}_\alpha \rho_\alpha X_\alpha^\kappa - D_{\alpha,pm}^\kappa \rho_\alpha \frac{M^\kappa}{\bar{M}_\alpha} \nabla x_\alpha^\kappa \right) h_\alpha^\kappa - \lambda_{T,pm} \nabla T \right) \cdot \mathbf{n} \right]^{pm}$$

530

531 The coupling condition for the energy balances may also include the net radiation R_n [$\text{J m}^{-2} \text{s}^{-1}$] as
 532 an additional energy flux to the porous medium. However, the assumption of thermal equilibrium
 533 may be violated in case of fast invasion of water with a different temperature or strong temperature
 534 differences between the free flow and porous medium [Nuske *et al.*, 2014].

535

536 **Simplifications and fixes:**

537 The exchange processes are closely linked to the geometry and the roughness of the interface
 538 which is not resolved in the abovementioned simulation models. The effect of this non-resolved
 539 geometry or roughness needs to be parameterized in the coupling conditions. In the following
 540 section, we discuss several simplifications that are made for coupling processes in the porous
 541 medium and the free flow.

542

543 **Full turbulence model and roughness**

544 For smooth surfaces, the effects of turbulence inside the viscous boundary layer are negligible.
 545 Therefore, the eddy coefficients approach zero and are not necessarily required in the coupling
 546 conditions.

547 For smooth surfaces, the roughness elements are covered with a viscous boundary layer, although
 548 the flow above the viscous layer may be turbulent. In this case the roughness influences the profile

of the eddy coefficients in the direction normal to the surface and thus the velocity profile and the viscous boundary layer thickness. Still, the coupling occurs in the viscous boundary layer. For rough surfaces, the height of the roughness elements is larger than the viscous layer thickness and the effects of the roughness and turbulence are important and cannot be neglected [Fetzer *et al.*, 2016]. This is accomplished by including the eddy coefficients, which are a function of roughness, in the coupling conditions above. In the section on one-dimensional transfer between the porous medium and the free flow, more details on the effect of roughness on the exchange processes are given.

Coupled one-dimensional transfer between the soil surface and free flow: aerodynamic resistances.

When lateral variations in wind, air temperature and humidity can be neglected, the sensible heat and vapor fluxes can be described as one-dimensional fluxes that are calculated using equivalent transfer resistances and differences in vapor concentrations and temperature that are measured at different heights but at the same horizontal location (e.g. [Monteith and Unsworth, 1990]):

$$H = c_a \frac{T(z = 0) - T(z_{ref})}{r_H} \quad [44]$$

$$F_w = \frac{\rho_g^w(z = 0) - \rho_g^w(z_{ref})}{r_V} \quad [45]$$

where H [$\text{J m}^{-2} \text{s}^{-1}$] is the sensible heat flux, c_a [$\text{J m}^{-3} \text{K}^{-1}$] is the volumetric heat capacity of moist air, z_{ref} (m) is a reference height at which wind speed, air temperature and air humidity are measured or defined, F_w [$\text{kg m}^{-2} \text{s}^{-1}$] is the water vapor flux, and r_H and r_V [s m^{-1}] are the aerodynamic resistance terms for vertical latent heat and vapor transfer in the air stream. Using a mass and energy balance at the soil surface, the vapor and sensible heat fluxes are linked to the water and vapor fluxes in the soil at the soil surface. The mass balance is given by:

$$F_w = \left[q_l \rho_l - D_{g,eff}^w(S_g) \frac{\partial \rho_g^w}{\partial z} \right]^{pm} \quad [46]$$

571

572 where the first and second terms on the right hand side are the liquid water and vapor flows towards
573 the soil surface, respectively.

574 For the energy balance equation at the soil surface, the solar and long wave radiation that is
575 absorbed by and emitted from the soil surface needs to be taken into account. Calling the sum of
576 these radiation terms the net radiation, R_n [$\text{J m}^{-2} \text{s}^{-1}$] (where positive radiation terms denote the
577 radiation that is absorbed and negative terms denote the radiation that is emitted), the energy
578 balance at the soil surface is:

$$H + h_g^w F_w - R_n = \left[-h_g^w D_{g,eff}^w(S_g) \frac{\partial \rho_g^w}{\partial z} + h_l^w \rho_l q_l - \lambda_{T,pm} \frac{\partial T}{\partial z} \right]^{pm} \quad [47]$$

579

580 Eqs. [44], [45], [46], [47] link the state variables, i.e. temperature and air vapor concentration, and
581 fluxes at the soil surface with state variables that are defined at the reference height in the air
582 stream. The latter may therefore be considered as Dirichlet boundary conditions for the water and
583 heat fluxes in the coupled soil-air system. This implies that the water and heat fluxes at the soil
584 surface can be derived from these prescribed state variables in the air stream and do not have to be
585 prescribed as flux boundary conditions.

586

587 Crucial parameters in Eqs. [44] and [45] are the aerodynamic resistance terms for vertical latent
588 and sensible heat transfer. They are related to the roughness of the soil surface, diffusive transfer
589 in the interfacial viscous or roughness layer, wind velocity and eddy diffusivity in the air stream,
590 and stability of the air above the heated soil surface. In the following discussion, we will consider
591 neutral stability conditions, i.e. the eddy diffusivity is not influenced by buoyancy. We refer the

592 reader to text books on meteorology (e.g. [Brutsaert, 1982; Monteith and Unsworth, 1990;
593 Shuttleworth, 2012]) for a detailed treatment of buoyancy effects.

594 In the air stream, a constant shear stress, τ_{turb} [N m⁻²], with height is assumed. τ_{turb} corresponds to
595 a momentum transfer from the air stream to the soil surface and can be expressed in terms of a
596 resistance equation similar to Eqs. [44] and [45]:

$$\tau_{turb} = \rho_g \frac{v_{g,x}(z_{ref}) - v_{g,x}(z = 0)}{r_M} \quad [48]$$

597
598 where $v_{g,x}$ [m s⁻¹] is the horizontal air velocity, and r_M [s m⁻¹] is the resistance for momentum
599 transfer between the reference height and the soil surface. r_M is derived from the vertical wind
600 profile in the ‘logarithmic/dynamic’ sublayer above the roughness layer.

601 Combining Eqs. [37], [38], and [48] leads to the following expression for r_M :

$$r_M = \frac{\ln\left(\frac{z}{z_{0m}}\right)}{v^* \kappa} = \frac{\left\{\ln\left(\frac{z}{z_{0m}}\right)\right\}^2}{v_{g,x}(z) \kappa^2} \quad [49]$$

602
603 The momentum roughness length, z_{0m} , is a function of the kinematic viscosity of air, ν , the friction
604 velocity, v^* , and the height and density of the roughness elements of the soil surface. For rough
605 surfaces z_{0m} depends only on the roughness of the surface. A prediction of z_{0m} based on the
606 geometry of the surface roughness seems to be very uncertain and Wieringa [1993] found that the
607 relationship between z_{0m} and the height of the surface roughness elements, d , may vary between:

$$z_{0m} = \frac{d}{100} \quad \text{and} \quad z_{0m} = \frac{d}{5} \quad [50]$$

608
609 For a small d or smooth surfaces, a viscous sublayer in which momentum transfer is dominated by
610 kinematic viscosity develops. In such a case, the velocity profiles and z_{0m} depend on v^* and ν :

$$z_{0m} = 0.135 \frac{\nu}{v^*} \quad [51]$$

611

612 Whether a surface is rough or (hydrodynamically) smooth depends on the roughness Reynolds

613 number, z_{0+} which is defined as:

$$z_{0+} = \frac{v^* z_{0m}}{\nu} \quad [52]$$

614

615 When $z_{0+} > 2$, the surface is considered to be rough whereas z_{0+} equals 0.135 for flat surfaces. It

616 should be noted that when z_{0m} is defined by $d/30$, the following well-known relation for a wind

617 speed profile above a rough surface is obtained [White, 1991]:

$$v_x(z) = \frac{v^*}{\kappa} \ln\left(\frac{z}{d}\right) + 8.5v^* \quad [53]$$

618

619 For smooth surfaces, the following relation is obtained:

$$v_x(z) = \frac{v^*}{\kappa} \ln\left(\frac{zv^*}{\nu}\right) + 5.0v^* \quad [54]$$

620

621 The transfer of water vapor and sensible heat in the logarithmic/dynamic sublayer is also caused

622 by turbulence and eddy diffusivity, which according to the Reynolds analogy may be considered

623 equivalent to the eddy viscosity. Therefore, a close relation between the transfer resistances for

624 momentum, sensible heat and vapor transfer may be assumed. Yet, these resistances differ from

625 each other because of the different transfer mechanisms in the viscous or roughness layer. The

626 kinematic air viscosity differs from the molecular diffusion of water and heat. Also, the roughness

627 of a bluff surface has a different effect on momentum transfer than on transfer of a scalar quantity

628 like vapor or sensible heat. For rough surfaces, momentum transfer can be considered more

629 effective or influential than vapor or heat transfer. Therefore the resistance for heat/vapor transfer

630 is larger than that for momentum transfer. As a consequence, an additional boundary resistance,

631 r_B [s m⁻¹] must be considered when relating the transfer resistances for vapor and sensible heat
 632 transfer to the momentum transfer:

$$r_V \approx r_H = r_M + r_B \quad [55]$$

633

634 The larger resistance results in a larger gradient of vapor and temperature across the viscous or
 635 roughness layer; the vapor and heat roughness lengths z_{0v} and z_{0H} are therefore smaller than z_{0m} .
 636 The similar transfer through the logarithmic/dynamic layer allows for the transfer resistance for
 637 vapor and heat transport to be described using an equation similar to Eq. [49]:

$$r_{V,H} = \frac{\ln\left(\frac{z}{z_{0v,H}}\right)}{v^* \kappa} = \frac{\left\{\ln\left(\frac{z}{z_{0v,H}}\right)\right\}^2}{v_{g,x}(z) \kappa^2} \quad [56]$$

638

639 This equation may be rewritten in terms of r_m and r_B as:

$$r_{V,H} = r_M + r_B = \frac{\ln\left[\frac{z}{z_{0v,H}}\right]}{\kappa v^*} = \frac{\ln\left[\frac{z}{z_{0m}}\right]}{\kappa v^*} + \frac{\ln\left[\frac{z_{0m}}{z_{0v,H}}\right]}{\kappa v^*} = \frac{\ln\left[\frac{z}{z_{0m}}\right]^2}{\kappa^2 v_{g,x}(z)} + \frac{\ln\left[\frac{z}{z_{0m}}\right] \ln\left[\frac{z_{0m}}{z_{0v,H}}\right]}{\kappa^2 v_{g,x}(z)} \quad [57]$$

640

641 A number of equations that relate $z_{0v,H}$ with z_{0m} and v^* have been proposed (see for instance
 642 *Yang et al.* [2008]). *Brutsaert* [1982] developed the following relation between z_{0m} and $z_{0v,H}$:

$$\frac{z_{0v,H}}{z_{0m}} = 7.4 \exp\left[-2.46 \left(\frac{v^* z_{0m}}{v}\right)^{0.25}\right] = 7.4 \exp\left[-2.46 \left(\frac{\kappa v_{g,x}(z) z_{0m}}{\ln\left(\frac{z}{z_{0m}}\right) v}\right)^{0.25}\right] \quad [58]$$

643

644 In Figure 2, the calculated resistances using Eq [49], [50], [57], and [58] for different surface
 645 roughness lengths, d and two wind velocities, $v_{g,x}$, at 2m height above the soil surface are shown.
 646 According to these calculations, the total resistance (r_H) decreases with increasing roughness. This
 647 can be attributed to the decreasing transfer resistance in the logarithmic/dynamic sublayer with
 648 increasing roughness of the soil surface. However, the difference between transfer resistance for

649 momentum transfer, r_M , and heat/vapor transfer, $r_{V,H}$ (i.e. r_B .) increases with increasing roughness.
650 For heat/vapor transfer, the effect of larger turbulent diffusivity in the logarithmic/dynamic layer
651 above a rougher soil surface is counteracted by a longer diffusive pathway through a thicker
652 roughness layer. As a consequence, the decrease of the resistance for heat/vapor transfer with
653 increasing surface roughness is less prevalent than the decrease of momentum transfer resistance
654 (Figure 2).

655 It should be noted that the transfer resistances described above are based on the assumption of a
656 bluff surface with a no-slip boundary condition. As described before, slip conditions may apply at
657 the surface of a porous medium, which can be accounted for by Beavers-Joseph interface boundary
658 conditions. One way to represent these effects is to define a displacement height, similar to what
659 is used to describe momentum, heat, and vapor transfer between vegetated surfaces and the
660 atmosphere. However, this displacement height should be negative. We are at this moment, not
661 aware of any studies that specify such displacement heights for air flow over rough dry porous
662 media.

663

664 **Semi-coupled porous medium and free flow using potential evaporation rates and soil** 665 **surface resistances for drying porous medium.**

666 In the sections above, we described how water flow and heat transport in the porous medium and
667 the free flow are coupled at the interface. However, this coupling is often relaxed by specifying or
668 defining state variables a-priori at the interface. When the vapor pressure at the interface is defined
669 to be the saturated vapor pressure, the water flux from the interface into the free flow is::

$$F_{w,pot} = \frac{\rho_{g,sat}^w(z=0) - \rho_g^w(z_{ref})}{r_V} \quad [59]$$

670 where $F_{w,pot}$ is the so-called potential evaporation, which is calculated without considering the
671 porous medium. It represents the ‘demand’ for water by the atmosphere and can be used as a flux
672 boundary condition in the porous medium as long as the flow in the porous medium can ‘supply’

673 the demand. The saturated vapor concentration at the soil surface depends on the soil surface
 674 temperature, which is derived from solving the surface energy balance (Eq. [47]). [ENREF 1](#)
 675 An additional soil transfer resistance, r_s [$s\ m^{-1}$] was introduced to account for a reduction in
 676 evaporation when the soil surface dries out and the vapor pressure becomes smaller than the
 677 saturated vapor pressure:

$$F_w = \frac{\rho_{g,sat}^w(z = z_{evap}) - \rho_g^w(z_{ref})}{r_v + r_s(\theta_{l,top})} = \beta(\theta_{l,top})F_{w,pot} \quad [60]$$

678
 679 where z_{evap} is the depth where evaporation takes place (i.e. where air is assumed to be saturated
 680 with vapor) and $\theta_{l,top}$ is the water content of the ‘top soil layer’. However, neither z_{evap} nor the
 681 thickness of the top soil layer are explicitly defined or simulated. The soil transfer resistance, r_s , is
 682 a function of the water content in the top soil layer whereas r_v depends on the free flow conditions.
 683 Water transport in the porous medium and into the atmosphere are hence semi-coupled in this
 684 approach. The β factor represents the ratio of the aerodynamic resistance to the sum of the soil and
 685 aerodynamic resistance. This approach is often used in large scale simulation models to describe
 686 the reduction of evaporation from drying bare soil compared with the potential evaporation from
 687 wet soil [*Tang and Riley*, 2013a].

688 *Kondo et al.* [1990], *Mahfouf and Noilhan* [1991], and *Vandegriend and Owe* [1994] used a soil
 689 transfer resistance term that increases with decreasing surface soil water content to account for the
 690 additional resistance for diffusive vapor transfer when the evaporative surface recedes into the soil
 691 profile and *Tang and Riley* [2013a] derived a model for the soil transfer resistance based on the
 692 vapor diffusivity and liquid water hydraulic conductivity. Experimentally derived soil transfer
 693 resistances were smaller than expected, considering the depth of the evaporation surface and the
 694 vapor diffusion coefficient. The smaller resistances were attributed to turbulent eddies that
 695 propagate into the porous medium and generate upward and downward movement of air and hence
 696 an extra opportunity for mixing with incoming air in the upper soil layer [*Farrell et al.*, 1966;

697 *Ishihara et al.*, 1992; *Kimball and Lemon*, 1971; *Scotter and Raats*, 1969]. It should be noted that
698 *Assouline et al.* [2013] found that the evaporation flux calculated using Ficks' Law and the depth
699 of the evaporation front (i.e. z_{evap}) underestimated the evaporation rate; however turbulent mixing
700 was not recognized in this case as a potentially relevant process. Additional turbulent mixing leads
701 to an additional dispersive flux of gases in the upper soil layer and has been shown to be of
702 importance for the flux of vapor and trace gases from soil [*Baldocchi and Meyers*, 1991; *Maier et*
703 *al.*, 2012; *Poulsen and Moldrup*, 2006] and soil covered with mulches [*Fuchs and Hadas*, 2011].
704 The parameterization of this additional mixing due to turbulence in the top soil is not well known
705 and debated.

706 A second reason for a decrease in evaporation rate from a drying surface is the spatial variation of
707 the vapor pressure at the soil surface at the microscopic scale. When the lateral distance between
708 evaporating water surfaces in pores at the soil surface becomes too large, the reduction of the
709 evaporating water surface when the soil surface dries out cannot be compensated by an increased
710 lateral diffusion of vapor through the viscous or roughness layer [*Haghighi et al.*, 2013;
711 *Shahraeeni et al.*, 2012; *Suzuki and Maeda*, 1968]. In this case, vapor transfer through the viscous
712 or roughness layer rather than vapor transfer within the porous medium is the limiting factor. If
713 this effect is also accounted for by an additional resistance term, experimental results of
714 *Shahraeeni et al.* [2012] suggest that this resistance term increases with decreasing surface soil
715 water content, that it is larger in soils with larger pores, and that the ratio of this resistance term to
716 the resistance for vapor transport from a saturated soil surface increases with increasing wind
717 velocity. It should be noted that a similar relation with wind speed is observed for the ratio of r_B/r_M
718 (see Figure 2).

719 Soil transfer resistances have been introduced in soil evaporation models. However, using an
720 additional transfer resistance in a model that explicitly considers diffusive vapor transfer in the
721 soil surface layer (e.g. *Saito et al.* [2006]) leads to a double counting of the transfer resistance

722 through the soil surface layer and therefore a too strong and rapid decrease in the actual
723 evaporation rate from the soil surface.

724

725 **Threshold formulation of boundary conditions.**

726 In this approach, water transfer between the porous medium and the free flow is either fully
727 controlled by free flow conditions or by water transport in the porous medium. When the free flow
728 controls the transfer, the potential evaporation is used as a flux boundary condition for water flow
729 in the porous medium. When the porous medium controls the flux, a constant water pressure or
730 water content at the surface of the porous medium is defined and the water flux towards the soil
731 surface is calculated by solving the flow equations in the porous medium for a Dirichlet boundary
732 condition. This approach is used in soil models that solve the Richards equation, e.g. Hydrus 1D
733 [Simunek *et al.*, 2008]. There are no exact guidelines to define the critical pressure head, ψ_{crit} ,
734 which is kept constant at the porous medium surface. As a rule of thumb, ψ_{crit} should correspond
735 with a pressure head for which the hydraulic conductivity and capacity of the porous medium
736 ($d\theta/d\psi$) become very small so that a smaller ψ_{crit} would hardly influence simulated water contents
737 and water fluxes towards the soil surface. As will be shown in some simulation examples in the
738 accompanying paper, simulated water fluxes are not so sensitive to the exact choice of this critical
739 pressure head.

740

741 **Summary and Conclusions:**

742 This work presented an overview of concepts with different complexity that can be used to describe
743 the transfer of water and energy from a porous medium into free flow. We identified how the
744 different approaches are related and which simplifications are used. The most comprehensive
745 description of processes considered multi-dimensional flow of liquid and gas phases and transport

746 of dry air and water components in the porous medium that was coupled consistently
747 acknowledging mechanical, chemical and thermal equilibrium at the interface to a free flow in the
748 gas phase and transport of vapor and heat above the porous medium. Since the direction of the free
749 flow is generally different from the main direction of the flow and transport processes in the porous
750 medium, this comprehensive approach implies a multi-dimensional description of the flow and
751 transport processes.

752 However, for homogeneous soil surfaces of a sufficiently large fetch, lateral variations in state
753 variables in the free flow become very small. This leads to a first simplification from a multi- to a
754 one dimensional description of the flow and transport processes in which only the vertical
755 components of flow and transport (in the porous medium) are considered and the vertical
756 components of the gas flow in both the porous medium and the free flow are neglected. This
757 implies that in the porous medium transport in the gas phase happens by diffusion only (i.e. air
758 flow is neglected). This assumption allows to couple the water and heat fluxes in the porous
759 medium and in the free-flow at the porous medium interface using transfer resistances that
760 calculate fluxes from states at the soil/free-flow interface and at a defined height in the free-flow.
761 A second simplification assumes that vapor transport in the porous medium can be neglected
762 leading to the one component one phase or so-called Richards equation. This simplification
763 decouples water from heat fluxes in the porous medium. At the porous-medium free flow interface,
764 the heat balance equation is solved to determine the water flux at the interface. This balance is
765 solved assuming that the vapor concentration at the soil surface is equal to the saturated vapor
766 concentration so that the heat balance equation is in fact decoupled from the water flow equation
767 in the porous medium. The water fluxes that are derived from this heat balance apply therefore
768 only when the soil surface is sufficiently wet.

769 The third set of simplifications is related to the description of the interactions or the coupling of
770 the water flow in the porous medium, the interface heat balance, and the evaporation from the
771 interface. In a first approach the transfer between the porous medium and free flow is described

772 by threshold boundary conditions that use prescribed fluxes derived from a surface energy balance
773 until a critical threshold water pressure head is reached at the porous medium surface. This so-
774 called Richards equation with threshold boundary conditions is widely used in soil water balance
775 models. During periods when the pressure head at the surface equals the critical pressure head, the
776 dynamics of the evaporation fluxes are completely defined by the hydraulic properties of the
777 porous medium and the water distribution in the porous medium but are decoupled from the
778 dynamics of the evaporative forcing: radiation, free flow velocity, relative humidity and
779 temperature. A second approach, which is often used in large scale simulation models, combines
780 the diurnal dynamics of the evaporation of a wet surface with a soil surface resistance depending
781 on the soil water content and represents a semi-coupling between the dynamics of the evaporative
782 forcing and the flow process in the porous medium.

783 Finally, there are processes that are not represented or resolved in the comprehensive process
784 description that we presented. These processes are parameterized in the vapor transport description
785 in the porous medium and in the transfer resistances for momentum, heat and vapor transfer
786 between the porous medium and the free flow. . Processes like turbulent diffusion and
787 enhancement of thermal vapor diffusion by thermal non-equilibrium within the porous medium
788 are parameterized in the vapor transport. Non-equilibria (thermal and chemical) can be included
789 in the models by adding additional equations that describe the rate with which an equilibrium is
790 reached, typically first-order rates [*Smits et al.*, 2011]. The rate coefficients are in essence
791 additional empirical parameters that need to be estimated, for example by inverse modeling. Since
792 the surface roughness is not represented in the continuum equations, the effect of roughness on the
793 exchange processes needs to be parameterized in the transfer resistances. Because the small scale
794 mechanisms that control the exchange processes at a rough interface differ for momentum vs heat
795 and vapor exchanges, the parameterizations of the respective transfer resistances differ. However,
796 these parameterizations have been derived mainly for bluff surfaces. Therefore, the effect of

797 vertical (turbulent pumping) and lateral gas flow in the surface layer of the porous medium, which
798 may be important in highly porous mulches, aggregated soils, and dry soils, is not accounted for.
799 Based on this summary, we conclude that the description of evaporation processes in systems
800 where an important lateral variation in fluxes and states can be expected would require a
801 multidimensional representation of the processes in both the porous medium and the free flow.
802 Although this seems at first sight trivial, it is in fact not generally applied. For instance, several
803 studies that investigated the effect of soil heterogeneity on soil water fluxes use a multidimensional
804 description of the flow process in the porous medium but describe the transfer from the soil surface
805 into the atmosphere using transfer resistances that presume laterally homogeneous state variables
806 in the free flow.

807 The consideration of the vapor transport in the porous medium and its parameterization due to
808 non-represented processes or its indirect representation in transfer resistances between the porous
809 medium and the free flow is another important difference between the presented model concepts.
810 Under which conditions these differences lead to important differences in simulated evaporation
811 needs to be further investigated.

812 These conclusions are the starting point of accompanying paper in which we will evaluate the
813 impact of lateral variability and the representation of vapor transport in the porous medium on
814 evaporation simulations.

815

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817

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823 comments and suggestions that have contributed to improve this paper.

824 **Tables:**

825 **Table 1: Overview of the equations that describe processes in the porous medium, the free flow, and the coupling conditions at the porous medium-free flow interface**
826 **using different degrees of simplifications.**

Porous medium equations			
2 component 2 phase	1 component 1.5 phase (nonisothermal)	1 component 1.5 phase (isothermal)	1 component 1 phase (Richards)
Component (dry air and water) and phase (gas and liquid) equations			
$\sum_{\alpha \in \{l,g\}} \phi \frac{\partial \rho_{\alpha} X_{\alpha}^{\kappa} S_{\alpha}}{\partial t} + \nabla \cdot \mathbf{F}^{\kappa} = 0$	$\phi \frac{\partial \rho_g X_g^w S_g}{\partial t} + \phi \frac{\partial \rho_l S_l}{\partial t} + \nabla \cdot \mathbf{F}^{\kappa} = 0$ <p>Equivalent formulation:</p> $\frac{\partial \theta_l}{\partial t} + \frac{\partial \theta_v}{\partial t} = \nabla \cdot \left[(\mathbf{K}_{l,\psi} + \mathbf{K}_{v,\psi}) \frac{\sigma(T)}{\sigma(T_{ref})} \nabla \psi _{T_{ref}} + \mathbf{K}_{l,\psi} \mathbf{e}_z \right]$ $+ \nabla \cdot (\mathbf{K}_{l,T} + \mathbf{K}_{v,T}) \nabla T$	$\frac{\partial \theta_v}{\partial t} + \frac{\partial \theta_l}{\partial t} =$ $\frac{\partial}{\partial z} \cdot \left[(\mathbf{K}_{l,\psi} + \mathbf{K}_{v,\psi}) \frac{\partial \psi}{\partial z} + \mathbf{K}_{l,\psi} \right]$	$\frac{\partial \theta_l}{\partial t} = \frac{\partial}{\partial z} \cdot \left[\mathbf{K}_{l,\psi} \frac{\partial \psi}{\partial z} + \mathbf{K}_{l,\psi} \right]$
$\mathbf{F}^{\kappa} = \sum_{\alpha \in \{l,g\}} \left(\mathbf{q}_{\alpha} \rho_{\alpha} X_{\alpha}^{\kappa} - D_{\alpha,pm}^{\kappa} \rho_{\alpha} \frac{M^{\kappa}}{\bar{M}_{\alpha}} \nabla x_{\alpha}^{\kappa} \right)$	$\mathbf{F}^w \approx \mathbf{q}_l \rho_l - \mathbf{D}_{g,pm}^w(S_g) \nabla \rho_g^w$		
$\mathbf{q}_{\alpha} = - \frac{k_{r\alpha}(S_{\alpha})}{\mu_{\alpha}} \mathbf{k} \cdot \nabla (p_{\alpha} - \rho_{\alpha} \mathbf{g} \cdot \mathbf{z})$	$\mathbf{q}_l = - \frac{k_{rl}(S_l)}{\mu_l} \mathbf{k} \nabla (p_l - \rho_l \mathbf{g} \cdot \mathbf{z})$		
Heat equations			
$\sum_{\alpha \in \{l,g\}} \phi \frac{\partial \rho_{\alpha} u_{\alpha} S_{\alpha}}{\partial t} + (1 - \phi) \frac{\partial \rho_s c_s T}{\partial t} + \nabla \cdot \mathbf{F}_T = 0$			
$\mathbf{F}_T = \sum_{\kappa \in \{a,w\}} \sum_{\alpha \in \{l,g\}} \left(\mathbf{q}_{\alpha} \rho_{\alpha} X_{\alpha}^{\kappa} - D_{\alpha,pm}^{\kappa} \rho_{\alpha} \frac{M^{\kappa}}{\bar{M}_{\alpha}} \nabla x_{\alpha}^{\kappa} \right) h_{\alpha}^{\kappa}$ $- \lambda_{T,pm} \nabla T$			

827
828

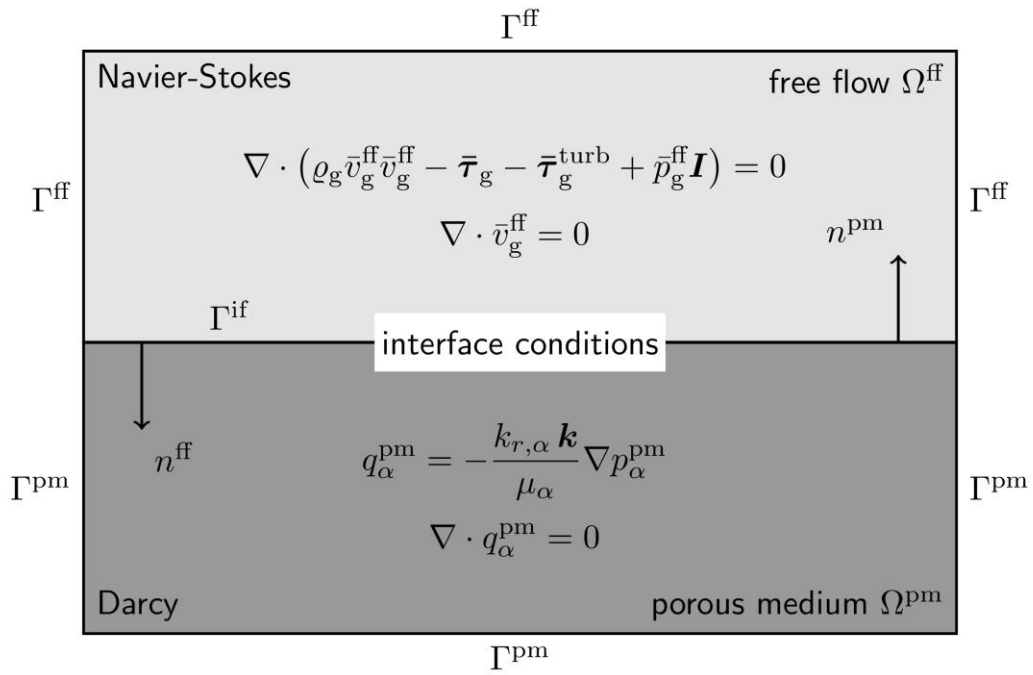
Free flow equations	
Mass balance, Reynolds averaged Navier Stokes, component and energy balance	1-D steady state
$\frac{\partial \rho_g}{\partial t} + \nabla \cdot [\rho_g \overline{\mathbf{v}_g}] = 0$	
$\frac{\partial (\rho_g \overline{\mathbf{v}_g})}{\partial t} + \nabla \cdot [\rho_g \overline{\mathbf{v}_g} \overline{\mathbf{v}_g} + \overline{p_g} \mathbf{I} - (\mu_g^{turb} + \mu_g)(\nabla \overline{\mathbf{v}_g} + \nabla \overline{\mathbf{v}_g}^T)] - \rho_g \mathbf{g} = 0$	$\frac{d}{dz} \mu_g^{turb} \frac{dv_{g,x}}{dz} = 0$
$\frac{\partial \rho_g \overline{X_g^\kappa}}{\partial t} + \nabla \cdot \left(\rho_g \overline{\mathbf{v}_g} \overline{X_g^\kappa} - (D_g^{turb} + D_g^\kappa) \rho_g \frac{M^\kappa}{M_g} \nabla \overline{x_g^\kappa} \right) = 0$	$\frac{d}{dz} D_g^{turb} \frac{d\rho_g^w}{dz} = 0$
$\frac{\partial \rho_g \overline{u_g}}{\partial t} + \nabla \cdot \left(\rho_g \overline{\mathbf{v}_g} \overline{h_g} - (\lambda_{T,g}^{turb} + \lambda_{T,g}) \nabla \overline{T} - \sum_{\kappa \in \{a,w\}} h_g^\kappa (D_g^{turb} + D_g^\kappa) \rho_g \frac{M^\kappa}{M_g} \nabla \overline{x_g^\kappa} \right) = 0$	$\frac{d}{dz} \lambda_{T,g}^{turb} \frac{dT}{dz} = 0$

829

830

Coupling conditions at the porous medium free flow interface			
2 component 2 phase	1-D transfer, aerodynamic resistances	Semi-coupled using soil surface resistance	Semi-coupled using threshold
Mechanical transfer			
$\left[\mathbf{n} \cdot \left(\{-\rho_g \mathbf{v}_g \mathbf{v}_g - \boldsymbol{\tau}_g - \boldsymbol{\tau}_g^{turb} + p_g \mathbf{I}\} \mathbf{n} \right) \right]^{ff} = [p_g]^{pm}$			
$\left[\left(\mathbf{v}_g + \frac{\sqrt{k_i}}{\alpha_{BJ} \mu_g} (\boldsymbol{\tau}_g + \boldsymbol{\tau}_g^{turb}) \mathbf{n} \right) \cdot \mathbf{t}_i \right]^{ff} = 0, \quad i \in \{1, \dots, d-1\}$	$\tau = \rho_g \frac{v_{g,x}(z_{ref}) - v_{g,x}(z=0)}{r_M}$ $r_M = \frac{z_{ref} \rho_g \ln\left(\frac{z_{ref}}{z_{0m}}\right)}{\mu_g^{turb}(z_{ref})}$		
Component transfer			
$[x_g^\kappa]^{ff} = [x_g^\kappa]^{pm}, \quad \kappa \in \{a, w\}$			
$\left[\left(\rho_g \mathbf{v}_g X_g^\kappa - (D_g + D_g^{turb}) \rho_g \frac{M^\kappa}{M_g} \nabla x_g^\kappa \right) \cdot \mathbf{n} \right]^{ff} = - \left[\left(\rho_g \mathbf{q}_g X_g^\kappa - D_{g,pm}^\kappa \rho_g \frac{M^\kappa}{M_g} \nabla x_g^\kappa + \rho_l \mathbf{q}_l X_l^\kappa - D_{l,pm}^\kappa \rho_l \frac{M^\kappa}{M_l} \nabla x_l^\kappa \right) \cdot \mathbf{n} \right]^{pm}$	$\frac{\rho_g^w(z=0) - \rho_g^w(z_{ref})}{r_v} = \left[q_l \rho_l - D_{g,eff}^w(S_g) \frac{\partial \rho_g^w}{\partial z} \right]^{pm}$ $r_v \approx r_H = r_M + r_B$	$\frac{\rho_{g,sat}^w(z=z_{evap}) - \rho_g^w(z_{ref})}{r_v + r_s(\theta_{l,top})} = [q_l \rho_l]^{pm}$	$\text{If } \psi(z=0) > \psi_{crit} \quad \frac{\rho_{g,sat}^w(z=0) - \rho_g^w(z_{ref})}{r_v} = [q_l \rho_l]^{pm}$ $\text{Else } \psi(z=0) = \psi_{crit}$
Heat transfer			
$[T]^{ff} = [T]^{pm}$			
$\left[\left(\rho_g h_g \mathbf{v}_g - (\lambda_{T,g} + \lambda_{T,g}^{turb}) \nabla T - \sum_{\kappa \in \{a,w\}} h_g^\kappa (D_g^\kappa + D_g^{turb}) \rho_g \frac{M^\kappa}{M} \nabla x_g^\kappa \right) \cdot \mathbf{n} \right]^{ff} = R_n - \left[\left(\sum_{\kappa \in \{a,w\}} \sum_{\alpha \in \{l,g\}} \left(\mathbf{q}_\alpha \rho_\alpha X_\alpha^\kappa - D_{\alpha,pm}^\kappa \rho_\alpha \frac{M^\kappa}{M_\alpha} \nabla x_\alpha^\kappa \right) h_\alpha^\kappa - \lambda_{T,pm} \nabla T \right) \cdot \mathbf{n} \right]^{pm}$	$c_a \frac{T(z=0) - T(z_{ref})}{r_H} + h_g^w \frac{\rho_g^w(z=0) - \rho_g^w(z_{ref})}{r_v} - R_n = \left[-h_g^w D_{g,eff}^w(S_g) \frac{\partial \rho_g^w}{\partial z} + h_l^w \rho_l q_l - \lambda_{T,pm} \frac{\partial T}{\partial z} \right]^{pm}$	$c_a \frac{T(z=0) - T(z_{ref})}{r_H} + h_g^w \frac{\rho_{g,sat}^w(z=z_{evap}) - \rho_g^w(z_{ref})}{r_v + r_s(\theta_{l,top})} - R_n = \left[h_l^w \rho_l q_l - \lambda_{T,pm} \frac{\partial T}{\partial z} \right]^{pm}$	$\text{If } \psi(z=0) > \psi_{crit} \quad c_a \frac{T(z=0) - T(z_{ref})}{r_H} + (h_g^w - h_l^w) \frac{\rho_{g,sat}^w(z=0) - \rho_g^w(z_{ref})}{r_v} - R_n = \left[-\lambda_{T,pm} \frac{\partial T}{\partial z} \right]^{pm}$ $\text{Else:} \quad c_a \frac{T(z=0) - T(z_{ref})}{r_H} - R_n = \left[(h_l^w - h_g^w) \rho_l q_l - \lambda_{T,pm} \frac{\partial T}{\partial z} \right]^{pm}$

832 **Figures:**



833

834 **Figure 1: Sketch of the two-domain concept and the notation of the normal vectors (after Mosthaf et al.**

835

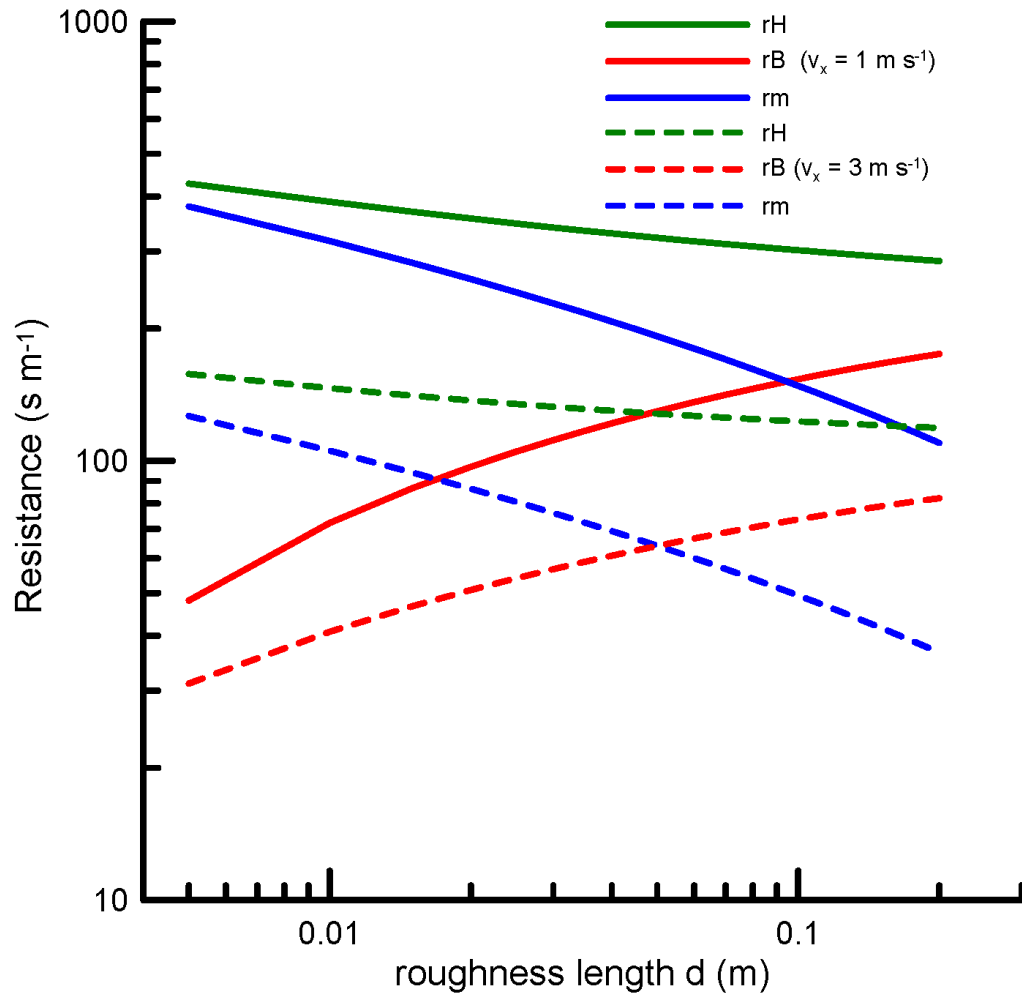


Figure 2: Aerodynamic resistances for sensible heat (and vapor) (r_H) and momentum transfer (r_m) through the boundary layer as function of the surface roughness length, d , for two different wind speeds, $v_{g,x}$ at 2 m height. r_B represents the additional resistance for heat transfer compared with momentum transfer.

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843

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